

# Quantum cosmology with big-brake singularity

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We investigate a cosmological model with a big-brake singularity in the future: while the first time derivative of the scale factor goes to zero, its second time derivative tends to minus infinity. Although we also discuss the classical version of the model in some detail, our main interest lies in its quantization. We formulate the Wheeler–DeWitt equation and derive solutions describing wave packets. We show that all such solutions vanish in the region of the classical singularity, a behaviour which we interpret as singularity avoidance. We then discuss the same situation in loop quantum cosmology. While this leads to a different factor ordering, the singularity is there avoided, too.

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## I. INTRODUCTION

It is a well-known fact that general relativity is an incomplete theory in the sense that solutions to Einstein’s equations can contain singularities. These are regions (outside spacetime) where the theory itself breaks down. According to the singularity theorems, the occurrence of such singularities is a generic feature of ‘physical’ solutions to Einstein’s equations.

One outlook on this problem is to consider a quantum theory of gravity as the necessary completion of general relativity [1]. Consequently, it is expected that such a quantum theory of gravity is in some sense (still to be specified) free of these singularities. Investigations to this end are usually carried out, not in the full quantum gravity candidate theories, but in reduced models. That is, one takes a specific solution (conventionally and pragmatically specified by some symmetry) to Einstein’s equations and in some way applies the quantization procedure of the full theory to the reduced model.<sup>1</sup> Prototypes for such symmetry-reduced models are black-hole spacetimes and cosmological spacetimes.

In our paper we restrict the discussion to cosmological models. Here, in the canonical approach, we have basi-

cally two candidates for a quantum cosmological theory: minisuperspace quantization in the framework of the geometrodynamical approach and loop quantum cosmology [1, 4, 5]. In both approaches, one has to investigate whether singularities ‘do not occur’. This implies that for each approach one has defined what the sentence ‘singularities do not occur’ means. To come to the point, for neither of the two theories a strict proof of the avoidance of singularities exists.

Both approaches describe the universe via a wave function on configuration space which has to be the solution of a constraint equation. The constraint equation is the quantized version of the Hamiltonian constraint. The difference between both approaches lies in the way this equation is quantized. In loop quantum cosmology, one uses a so-called polymer representation instead of the conventional Schrödinger representation. This is done in analogy to the full theory. This procedure carried out in a naive way, leads to a difference equation in steps of a smallest length  $\mu_0$ . In geometrodynamics, one arrives at a differential equation, the Wheeler–DeWitt equation. In the continuum limit,  $\mu_0 \rightarrow 0$  (suitable conditions on the higher derivatives of the wave function implied), the loop quantum cosmological difference equation fades into the Wheeler–DeWitt equation [6].

Recently, Ashtekar *et al.* [7, 8] extended the ansatz using  $\mu_0$ , replacing it by  $\bar{\mu}$ , which is a function of the densitized triad operator  $\hat{p}$ . The equation is then a difference equation in eigenvalues  $v$  of the volume operator, and the Wheeler–DeWitt equation follows in the continuum limit for large volume. The factor-ordering of the Wheeler–DeWitt equation then does depend on the factor-ordering chosen for the difference equation. In [6] and [7, 8] different factor-orderings have been chosen. The two difference equations, in  $\mu_0$  or  $\bar{\mu}$ , can be under-

<sup>1</sup> A counter-example is causal dynamical triangulation [1, 2]. Here exists the possibility to reduce the full quantum theory by integrating out all degrees of freedom except the scale factor. The resulting theory yields an action differing from the geometrodynamical minisuperspace action by an overall minus sign in the realm where the continuum limit is valid. Numerical evaluation predicts a closed universe undergoing a bounce upon reaching small scales. Moreover, quantum spacetime on these scales is predicted to be of fractal structure and dimension 2, coinciding with results obtained in the asymptotic-safety approach [1, 3].

stood in a broader context as implementing different actions of the full Hamiltonian constraint. They are thus just two special cases of a wider class of constraints that might arise, the actual form of which should in principle be determined by the full Hamiltonian constraint, [9]. Whereas in the first case, the coordinate edge length of a holonomy is fixed and does not depend on the scale factor, in the second case it does. This can be interpreted as an implementation of the fact that in the full theory, the Hamiltonian constraint (whatever its exact form may be) creates vertices (in addition to changing the edge labels of the existing edges). As new vertices are created, the edge lengths decrease. The altered dynamics using  $\bar{\mu}$  then corresponds to a lattice in which the number of vertices grows linearly with volume.

In loop quantum cosmology, results on singularity resolution fall into one of three categories, [11]. As a first result one may quote that, in the isotropic case, the evolution equation is well-defined also on an evolution across the singularity. This is due to the discreteness of the evolution parameter which is a feature inherited from the full theory through the use of the polymer representation, [10]. This allows to evolve a wave packet, starting from any initial state, deterministically across the singularity, [13].

A second hint on singularity avoidance, so far studied in isotropic models with massless scalar field  $\phi$ , curvature index  $\mathcal{K} = 0, 1$  and zero as well as non-zero cosmological constant, is the occurrence of a so-called ‘bounce’. As a bounce one describes a deviation from the classical behaviour such that a semi-classical wave packet starting on a classical trajectory for large scale-factor deviates from this trajectory upon approach of the classical singularity and instead avoids the region of configuration space where the singularity is located. Here, avoidance refers to an exponential fall-off (in  $\phi$ ) of the wave function, [6, 7, 8].

A third criterium is given by the boundedness of the expectation value of the operator corresponding to the inverse scale factor. As the inverse scale factor is related to the curvature in isotropic, homogeneous models, this hints at avoidance of the curvature singularity. This is a feature which follows from the use of holonomies as basic variables. It is a purely kinematical result as the expectation value is evaluated with respect to states from the kinematical Hilbert space, [12, 13].

The robustness of these results is disputable to differing degree. Whereas the possibility to evolve the wave packet through singularities in a well-defined way seems to persist in the full theory, this is not so clear for the other two criteria.

The boundedness of the inverse scale factor seems to carry over to the full theory only when evaluated on a

subspace of the kinematical Hilbert space, [14]. Moreover, the occurrence of a bounce seems to be knit to isotropic models and even there it is not clear whether it should persist for more general settings involving a matter potential. The underlying concept in the models studied in this context is to use the scalar field as a ‘time’ variable (emergent time) with respect to which the wave packet is evolved (numerically). Transferring this concept to more general models including a scalar-field potential, one has to cope with a ‘time’ (i.e.  $\phi$ -) dependent evolution operator which is given by the square-root of the gravitational Hamiltonian plus the scalar field potential energy. It can therefore be arbitrarily complicated. In addition to that, it is not clear that  $\phi$  defines a ‘good clock’ throughout the universe evolution. The advantage of this approach, on the other hand, is the existence of an inner product which is uniquely defined by a complete set of Dirac observables, and thus provides expectation values of observables. Most importantly, the inner product supplies the model with a probability interpretation (even though no connection to the measurement process is made).

In the geometrodynamical framework, several models have been investigated regarding their ability to resolve the singularity problem. In this setting, singularity avoidance is defined as either a vanishing of the wave function at the point of the classical singularity<sup>2</sup> or a spreading of semi-classical states denoting a break-down of semi-classical concepts in general (the end of the world as we know it). In the semi-classical regime, an approximate Schrödinger equation can be derived from a WKB-expansion defining a notion of time [1]. This time label is necessary to stack together the 3-hypersurfaces on which the wave function has support. The thus obtained 4-dimensional spacetime can now be probed for geodesic completeness. Only in semi-classical regimes a notion of geodesics exists, and thus we can speak of the existence of singularities — in the strict mathematical sense of the singularity theorems — only there.

Accepting both criteria, singularity avoidance was found for big-bang/big-crunch singularities in various models (different scalar field potentials, cosmological constant, etc.) and for the big-rip singularity occurring at large scale factor, [15]. The big-rip singularity is a singularity which the universe can encounter when it ex-

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<sup>2</sup> More generally, it would be sufficient to demand that the probability vanishes there; for example, the ground-state wave function for the hydrogen atom, as found as a solution to the Dirac equation, diverges for  $r \rightarrow 0$ , but the probability there is zero because of the  $r^2$ -contribution from the measure. In quantum cosmology, this question is more subtle because the fundamental measure is not known [1].

pands “too rapidly” [16]. This singularity occurs when the cosmological radius of the universe  $a(t)$  tends to infinity at some finite moment of time simultaneously with its time derivative  $\dot{a}(t)$  in such a way that the Hubble variable  $H(t) \equiv \dot{a}/a$  tends to infinity as well. Interest in this type of singularity is connected with the fact that it arises quite naturally in cosmological models with phantom dark energy, that is, dark energy such that the equation of state parameter  $w = p/\rho < -1$  [17, 18], where  $p$  and  $\rho$  denote pressure and energy density of the cosmological fluid, respectively.

In the following, we want to analyze whether the so-called *big-brake singularity* can be avoided in a similar way. The big brake belongs to another class of cosmological singularities not connected with the divergence of the Hubble variable itself but of one of its higher derivatives. Singularities of this type are called soft, quiescent, or sudden [19, 20, 21]. These singularities occur at finite value of the scale factor and its time derivative and hence of the Hubble parameter, while the first or higher derivatives of the Hubble parameter are divergent, which implies divergence of some curvature invariants. The big brake is a special example for a model from this class; it was first considered in [22] (see there the discussion after Eq. (2.13)) and later discussed in detail in [21]. It can arise in tachyonic cosmological models [23] with a particular potential: at some finite moment of the cosmological evolution the universe stops at finite value of its cosmological radius with an infinite deceleration  $\ddot{a} \rightarrow -\infty$ . It was also noticed that the big-brake singularity can arise in more simple cosmological models, such as a universe filled with a perfect fluid obeying the equation of state  $p = A/\rho$ , where  $A$  is a positive constant. This equation of state was considered in [24] in the context of wiggly strings (these are cosmic strings with small-scale wiggles imposed on their dynamics). A fluid obeying this equation of state can be called “anti-Chaplygin” gas in analogy with the gas with Chaplygin equation of state  $p = -A/\rho$ , which has acquired some popularity in cosmology as candidate for unifying dark energy and dark matter [25, 26]. Independent of the possible relevance of such a model for the real Universe, it has the merit of showing that intriguing features can occur in the quantum version, connected with the presence of a quantum phase at large (instead of small) scale factor. Quantum effects at large cosmological scales have previously been studied in the context of a classically recollapsing quantum universe [27, 28].

Our paper is organized as follows: In Sec. II we present a simple classical model exhibiting a big-brake singularity. In Sec. III the Wheeler–DeWitt equation for this model is studied and approximate solutions describing wave packets are found. Their behaviour demonstrates

that the classical singularity is avoided. Sec. IV contains a discussion of the big-bang singularity. Sec. V makes a comparison with the description of this model in loop quantum cosmology. Sec. VI contains a discussion and an outlook. Some technical details are relegated to an appendix.

## II. THE CLASSICAL BIG-BRAKE MODEL

We consider a flat Friedmann–Lemaître universe filled with a perfect fluid mimicked by a homogeneous scalar field. We require the fluid to obey an “anti-Chaplygin” equation of state  $p = A/\rho$ , where  $p$  is the fluid pressure and  $\rho$  its energy density. In terms of the scalar field, these read

$$p = \frac{\dot{\phi}^2}{2} - V(\phi), \quad \rho = \frac{\dot{\phi}^2}{2} + V(\phi). \quad (1)$$

The corresponding action is

$$S = \frac{3}{\kappa^2} \int dt N \left( -\frac{a\dot{a}^2}{N^2} + \mathcal{K}a - \frac{\Lambda a^3}{3} \right) + \frac{1}{2} \int dt N a^3 \left( \frac{\dot{\phi}^2}{N^2} - 2V(\phi) \right), \quad (2)$$

where  $\kappa^2 = 8\pi G$ ,  $N$  is the lapse function,  $\Lambda$  the cosmological constant,  $V(\phi)$  a potential of the field  $\phi$ , and  $\mathcal{K} = 0, \pm 1$  is the curvature index; we set  $c = 1$ . Furthermore, we set  $N = 1$ , so the time parameter is the standard Friedmann cosmic time. The action then becomes

$$S = \frac{3}{\kappa^2} \int dt \left( -a\dot{a}^2 + \mathcal{K}a - \frac{\Lambda}{3}a^3 \right) + \frac{1}{2} \int dt \left( a^3\dot{\phi}^2 - 2a^3V(\phi) \right). \quad (3)$$

The canonical momenta are given by

$$\pi_a = -\frac{6a\dot{a}}{\kappa^2}, \quad \pi_\phi = a^3\dot{\phi}. \quad (4)$$

The canonical Hamiltonian  $\mathcal{H}$ , which is constrained to vanish, reads

$$\mathcal{H} = -\frac{\kappa^2}{12a}\pi_a^2 + \frac{\pi_\phi^2}{2a^3} + a^3\frac{\Lambda}{\kappa^2} + a^3V - \frac{3\mathcal{K}a}{\kappa^2} = 0. \quad (5)$$

In the following, we restrict the analysis to flat cosmologies,  $\mathcal{K} = 0$ , without cosmological constant,  $\Lambda = 0$ . The

Hamiltonian constraint yields the Friedmann equation

$$H^2 = \frac{\kappa^2}{3} \rho = \frac{\kappa^2}{3} \left( \frac{\dot{\phi}^2}{2} + V(\phi) \right). \quad (6)$$

The fluid obeys a continuity equation,

$$\dot{\rho} = -3H(\rho + p), \quad (7)$$

which in terms of the scalar field reads

$$\ddot{\phi} + 3H\dot{\phi} + \frac{dV}{d\phi} = 0. \quad (8)$$

Using the equation of state,  $p = A/\rho$ , (7) can be easily solved for  $\rho$  in terms of the scale factor,

$$\rho(a) = \sqrt{\frac{B}{a^6} - A}, \quad (9)$$

where  $B > 0$  is some integration constant, and we have chosen the solution with  $\rho \geq 0$ . Note that  $\rho$  is well defined only for  $a < a_* \equiv (B/A)^{1/6}$ , cf. Figure 1. As  $a_*$  is approached, the density goes to zero. We note that  $B$  has dimension mass squared, and  $A$  has dimension mass squared over length to the sixth power.

Using the result (9), one gets from (6):

$$\int_a^{a_*} \frac{d\tilde{a}}{\left(\frac{B}{\tilde{a}^2} - A\tilde{a}^4\right)^{\frac{1}{4}}} = \frac{\kappa}{\sqrt{3}}(t_0 - t), \quad (10)$$

where  $a(t_0) = a_*$  (“big brake”) and  $a(0) = 0$  (“big bang”). In order to calculate this integral, we substitute  $z = (B/a^6 - A)^{1/4}$ , with  $0 \leq z \leq \infty$ . Then (10) becomes

$$\int_0^z d\tilde{z} \frac{\tilde{z}^2}{\tilde{z}^4 + A} = \frac{\kappa\sqrt{3}}{2}(t_0 - t). \quad (11)$$

The integral on the left-hand side can be found in [29]. For (11) one then gets

$$\frac{1}{4A^{1/4}\sqrt{2}} \left( \ln \frac{z^2 - A^{1/4}z\sqrt{2} + A^{1/2}}{z^2 + A^{1/4}z\sqrt{2} + A^{1/2}} + 2 \arctan \frac{A^{1/4}z\sqrt{2}}{A^{1/2} - z^2} + \pi \theta(z^2 - A^{1/2}) \right) \quad (12)$$

$$= \frac{\kappa}{\sqrt{3}}(t_0 - t). \quad (13)$$

We have added the Heaviside  $\theta$ -function in order to make the arctan-function continuous at the point  $z^2 = A^{1/2}$ .

For the total time that elapses from big bang to big brake one then gets

$$t_0 = \frac{2}{\kappa\sqrt{3}} \int_0^\infty dz \frac{z^2}{z^4 + A} = \frac{\pi}{\sqrt{6}\kappa A^{1/4}} \quad (14)$$

The solution for  $a(t)$  is shown in Figure 2. A simple approximate solution can be found in the vicinity of  $a_*$ . To this end, we write  $a = a_* - \Delta a$ , which simplifies the above integral to

$$\int_0^{\Delta a} d\Delta a \frac{1}{a_*(6\Delta a)^{\frac{1}{4}}} = \sqrt{\frac{\kappa^2}{3}}(t - t_0), \quad (15)$$

yielding

$$\Delta a(t) = [C(t_0 - t)]^{\frac{4}{3}}. \quad (16)$$

So we find for the scale factor and its derivatives

$$a(t_0) = a_*, \quad \dot{a}(t_0) = 0, \quad \ddot{a}(t_0) = -\infty. \quad (17)$$

At  $t_0$ , the evolution of the scale factor comes to a halt. Its ‘speed’ is zero due to an infinite negative acceleration. It is this peculiar feature that gave the singularity its name, big-brake singularity.

The first and second time derivatives of the scale factor in terms of the scale factor itself are given by simple expressions. To this end, note that (10) can be differentiated with respect to  $a$ , thus connecting  $\dot{a}(t)$  with the scale factor according to

$$\frac{da}{dt} = \sqrt{\frac{\kappa^2}{3}} a \left( \frac{B}{a^6} - A \right)^{\frac{1}{4}}, \quad (18)$$

cf. Figure 3. Obviously, as  $a \rightarrow a_*$ ,  $\dot{a} \rightarrow 0$ . Differentiating again with respect to time, one finds

$$\frac{d^2a}{dt^2} = \frac{\kappa^2}{3} a \left( \frac{B}{a^6} - A \right)^{\frac{1}{2}} \left[ 1 - \frac{B}{4a^6} \left( \frac{B}{a^6} - A \right)^{-1} \right], \quad (19)$$

showing that  $\ddot{a}(t) \rightarrow -\infty$  as  $a \rightarrow a_*$ , cf. Figure 4.

What remains to be found, is an equation for  $\phi$ . As we are interested in the quantum model, the solution in configuration space,  $\phi(a)$ , suffices. This is obtained from

$$\dot{\phi}^2 = \rho + p, \quad (20)$$

using the equation of state and the Friedmann equation (6). The (exact) solution is

$$\phi_{\mp}(a) = \mp \sqrt{\frac{1}{3\kappa^2}} \operatorname{artanh} \left( \sqrt{1 - \frac{Aa^6}{B}} \right), \quad (21)$$

cf. Figure 5. This is only consistent if the potential is chosen to be

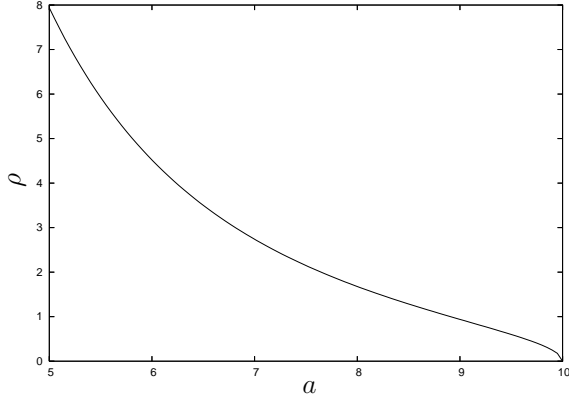


FIG. 1: Evolution of the energy density  $\rho$  of the scalar field with scale factor  $a$ .

$$V(\phi) = V_0 \left( \sinh(\sqrt{3\kappa^2}|\phi|) - \frac{1}{\sinh(\sqrt{3\kappa^2}|\phi|)} \right). \quad (22)$$

Given the trajectories  $\phi(a)$  and  $a(t)$ , the latter in explicit form only in the vicinity of the singularity, the classical model is thus fully described. Note that  $V_0 = \sqrt{A/4}$ . From (14) we find for the total lifetime of this model universe the expression

$$t_0 \approx 7 \times 10^2 \frac{1}{\sqrt{V_0 \left[ \frac{\text{g}}{\text{cm}^3} \right]}} \text{ s}. \quad (23)$$

This lifetime is much bigger than the current age of our Universe if

$$V_0 \ll 2.6 \times 10^{-30} \frac{\text{g}}{\text{cm}^3},$$

which is, of course, a reasonable result because the critical value of  $V_0$  just corresponds to the scale of the observed dark-energy density.

### III. THE QUANTUM BIG-BRAKE MODEL

#### A. Wheeler–DeWitt equation

Quantization is carried out in the canonical approach. Implementing the Hamiltonian constraint via Dirac’s constraint quantization, one arrives at the Wheeler–DeWitt equation

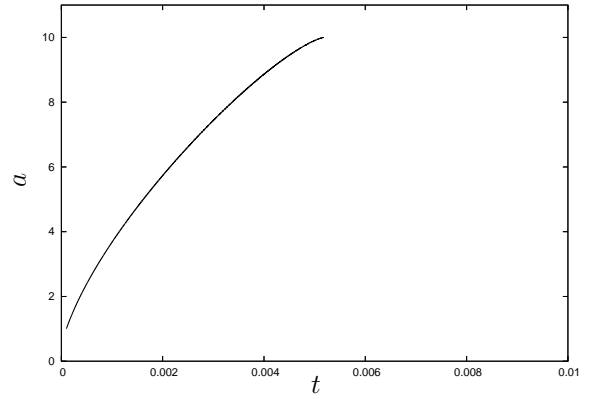


FIG. 2: Evolution of the scale factor over cosmic Friedmann time  $t$ .

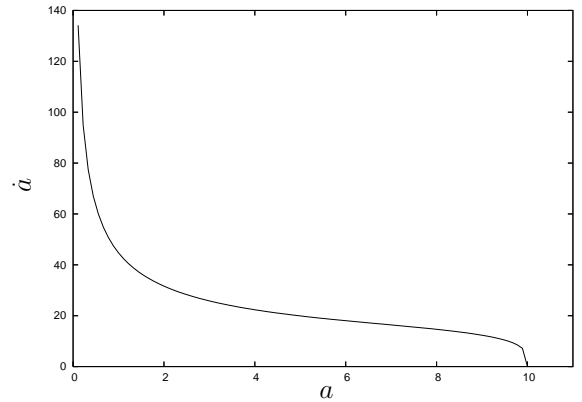


FIG. 3: Dependence of the derivative of the scale factor on the scale factor itself.

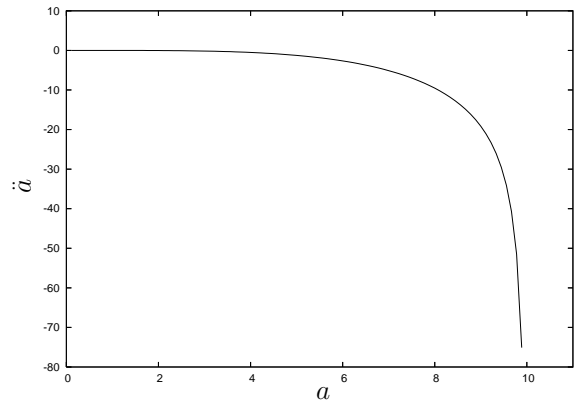


FIG. 4: Cosmic acceleration depicted over  $a$ .

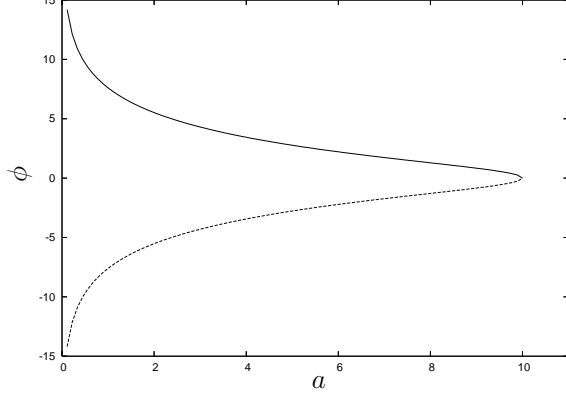


FIG. 5: Classical trajectory in configuration space.

$$\begin{aligned}
& \frac{\hbar^2}{2} \left( \frac{\kappa^2}{6} \frac{\partial^2}{\partial \alpha^2} - \frac{\partial^2}{\partial \phi^2} \right) \Psi(\alpha, \phi) \\
& + V_0 e^{6\alpha} \left( \sinh(\sqrt{3\kappa^2}|\phi|) - \frac{1}{\sinh(\sqrt{3\kappa^2}|\phi|)} \right) \Psi(\alpha, \phi) \\
& = 0,
\end{aligned} \tag{24}$$

where  $\alpha \equiv \ln a$  and the Laplace–Beltrami factor ordering has been employed. As we are interested in the behaviour in the vicinity of the big-brake singularity, where  $\phi$  is small, it is sufficient to approximate the potential there. We find

$$\frac{\hbar^2}{2} \left( \frac{\kappa^2}{6} \frac{\partial^2}{\partial \alpha^2} - \frac{\partial^2}{\partial \phi^2} \right) \Psi(\alpha, \phi) - \frac{\tilde{V}_0}{|\phi|} e^{6\alpha} \Psi(\alpha, \phi) = 0, \tag{25}$$

where  $\tilde{V}_0 = V_0/3\kappa^2$ .

### B. Born–Oppenheimer approximation to the Wheeler–DeWitt equation

Equation (25) can be solved, at least approximately, making the ansatz  $\Psi(\alpha, \phi) = \sum_k C_k(\alpha) \varphi_k(\alpha, \phi)$ , where  $\varphi_k(\alpha, \phi)$  is the solution of

$$-\left( \frac{\hbar^2}{2} \frac{\partial^2}{\partial \phi^2} + \frac{\tilde{V}_0}{|\phi|} e^{6\alpha} \right) \varphi_k(\alpha, \phi) = E_k(\alpha) \varphi_k(\alpha, \phi), \tag{26}$$

cf. also [30], where a similar ansatz was made. We recognize that this is the radial part of the time-independent Schrödinger equation for a particle in a Coulomb potential with  $l = 0$  and the wave function  $r\varphi_k$ . Thus, the

normalizable solutions are given by

$$\varphi_k(x_k) = N_k x_k e^{-\frac{x_k}{2}} L_{k-1}^1(x_k), \tag{27}$$

where  $x_k = 2\sqrt{-\frac{2E_k(\alpha)}{\hbar^2}}|\phi|$ , and  $L_{k-1}^1(x_k)$  denote the associated Laguerre polynomials;  $N_k = 1/k^{\frac{3}{2}}$  is the normalization factor;  $k \in \mathbb{N}$

The choice of the normalizable solution to (26) is enforced through the condition on the wave function imposed for large  $|\phi|$ , cf. Sec. IV D. The exact normalizable solution to (26) with the exact potential possesses a discrete spectrum; coincidence with the behaviour at small  $|\phi|$  is thus only achieved if the normalizable solution (27) is selected because the non-normalizable solutions have a continuous spectrum.

Note that  $\varphi_k(x_k) \rightarrow 0$  for  $|\phi| \rightarrow 0$ , since  $L_{k-1}^1(0) = k$ . To simplify notation, introduce  $Z(\alpha) \equiv \hbar^2/V_\alpha$  and  $V_\alpha \equiv \tilde{V}_0 e^{6\alpha}$ . Then,  $x_k = 2|\phi|/Z(\alpha)k$ . The functions  $\varphi_k(x_k)$  are orthogonal such that<sup>3</sup>

$$\int d\phi \varphi_k(x_k) \varphi_l(x_l) = Z(\alpha) \delta_{kl}. \tag{28}$$

The energy eigenvalues are

$$E_k(\alpha) = -\frac{V_\alpha^2}{2\hbar^2 k^2}. \tag{29}$$

Inserting this ansatz in (25) and carrying out a Born–Oppenheimer approximation, the resulting equation for  $C_k(\alpha)$  becomes

$$\ddot{C}_k(\alpha) - \frac{6V_\alpha^2}{\hbar^4 k^2 \kappa^2} C_k(\alpha) = 0, \tag{30}$$

where dots denote derivatives with respect to  $\alpha$ . Thus  $C_k$  is given by

$$C_k(\alpha) = c_1 I_0 \left( \frac{1}{\sqrt{6}} \frac{V_\alpha}{\hbar^2 k \kappa} \right) + c_2 K_0 \left( \frac{1}{\sqrt{6}} \frac{V_\alpha}{\hbar^2 k \kappa} \right), \tag{31}$$

where  $I_0, K_0$  denote modified Bessel functions of first and second kind, respectively. As a boundary condition, we require that the solution should vanish in the classically forbidden region,  $a > a_*$ . Therefore,  $c_1 = 0$  and only the MacDonald function  $K_0$  remains as solution. On the level of the Born–Oppenheimer approximation, the complete solution is therefore given by

<sup>3</sup> The validity of this relation is clear from the property of the  $\varphi_n$  being eigenfunctions of a Hermitian operator; its direct verification is discussed in [31].

$$\Psi(\alpha, \phi) = \sum_{k=1}^{\infty} A(k) N_k K_0 \left( \frac{1}{\sqrt{6}} \frac{V_\alpha}{\hbar^2 k \kappa} \right) \times \left( 2 \frac{V_\alpha}{k} |\phi| \right) e^{-\frac{V_\alpha}{k|\phi|}} L_{k-1}^1 \left( 2 \frac{V_\alpha}{k} |\phi| \right). \quad (32)$$

### C. Derivation of classical equations of motion from the principle of constructive interference

To derive a phase from this expression, approximate (26) and (30) further by a WKB-approximation. Making the ansatz  $\varphi_k(\alpha, \phi) = e^{\frac{i}{\hbar} S_{k0}^\phi(\alpha, \phi)}$  in (26),  $C_k(\alpha) = e^{\frac{i}{\hbar} S_{k0}^\alpha(\alpha)}$  in (30), one obtains to zeroth order in  $\hbar$  the Hamilton–Jacobi equation for the  $\phi$ - and  $\alpha$ -part, respectively. Integration yields for  $S_{k0}^\phi(\alpha, \phi)$ :

$$S_{k0}^\phi(\alpha, \phi) = \hbar k \left[ \arcsin \left( 1 - \frac{V_\alpha |\phi|}{\hbar^2 k^2} \right) - \frac{\pi}{2} \right] - \sqrt{2V_\alpha |\phi|} \sqrt{1 - \frac{V_\alpha |\phi|}{2\hbar^2 k^2}} - \frac{\pi}{4}, \quad (33)$$

in which the Langer boundary condition at the  $\alpha$ -dependent turning point  $\phi_t(\alpha) = 2\hbar^2 k^2 / V_\alpha$  has been employed. From (30), no phase results. This coincides with the limit  $\hbar \rightarrow 0$  in (31), as  $\lim_{x \rightarrow \infty} K_0(x) \approx \sqrt{\frac{\pi}{2x}} e^{-x}$ . So  $S_{k0}^\phi(\alpha, \phi)$  constitutes the entire phase.

The classical equations of motion should follow from the phase through the principle of constructive interference,  $\frac{\partial S_{k0}^\phi}{\partial k}|_{k=\bar{k}} = 0$ :

$$\begin{aligned} \frac{\partial S_{k0}^\phi}{\partial k}|_{k=\bar{k}} &= \hbar \left[ \arcsin \left( 1 - \frac{V_\alpha |\phi|}{\hbar^2 k^2} \right) - \frac{\pi}{2} \right] \\ &+ \frac{\sqrt{2V_\alpha |\phi|}}{k} \sqrt{1 - \frac{V_\alpha |\phi|}{2\hbar^2 k^2}} \\ &\stackrel{!}{=} 0, \end{aligned} \quad (34)$$

Here,  $\bar{k} = \sqrt{\frac{\tilde{V}_0}{\sqrt{3\kappa^2}} \frac{a_*^3}{\hbar}}$ . This constant arises under the conditions that, firstly,  $k$  and so also  $\bar{k}$  have to be dimensionless, and that, secondly, the only constants of the model are  $V_0$  (or  $\tilde{V}_0$ ),  $a_*$  (or  $A$  and  $B$ ),  $\hbar$  and  $\kappa$ . With this choice, (34) simplifies to

$$\begin{aligned} \frac{\partial S_{k0}^\phi}{\partial k}|_{k=\bar{k}} &= \hbar \left[ -\arccos \left( 1 - \left( \frac{a}{a_*} \right)^6 |\phi| \right) \right. \\ &\left. + \left( \frac{a}{a_*} \right)^3 \sqrt{2|\phi| - \left( \frac{a}{a_*} \right)^6 \phi^2} \right]. \end{aligned} \quad (35)$$

For the classical trajectory, (21), this is

$$\begin{aligned} \frac{\partial S_{k0}^\phi}{\partial k}|_{k=\bar{k}} &= \hbar \left[ -\arccos \left( 1 - \frac{|\phi|}{\cosh^2(\sqrt{3\kappa^2}|\phi|)} \right) \right. \\ &\left. + \frac{\sqrt{|\phi|}}{\cosh(\sqrt{3\kappa^2}|\phi|)} \sqrt{2 - \frac{|\phi|}{\cosh^2(\sqrt{3\kappa^2}|\phi|)}} \right]. \end{aligned} \quad (36)$$

But the classical equation of motion was derived using the full potential. The quantum theory uses an approximation to the original potential which is valid up to order  $\mathcal{O}(|\phi|^{\frac{3}{2}})$  for small  $\phi$ . Applying the same approximation to (36), one finds

$$\frac{\partial S_{k0}^\phi}{\partial k}|_{k=\bar{k}} = \hbar \mathcal{O}(|\phi|^{\frac{3}{2}}), \quad (37)$$

and so the classical solution (21) satisfies the condition for constructive interference with the above choice for  $\bar{k}$  for small  $\phi$ , which is consistent with the approximation of the potential in (25).

There is, of course, also the question whether the Born–Oppenheimer approximation employed in the last subsection is a feasible approximation. We show in Appendix A that this approximation is fulfilled in the limit  $a \rightarrow a_*$ , which is just the region under consideration here.

### D. Singularity avoidance

Wave packets in quantum cosmology have been constructed in order to study aspects of the quantum-to-classical correspondence, in particular the validity of the semi-classical approximation [1, 30, 32]. They are also useful in order to provide a consistent picture of the pre-big-bang to post-big-bang transition in quantum string cosmology [33]. Such a construction is also useful in the study of singularity avoidance.

Wave packets constructed from the solutions of (25) are of the general form

$$\Psi(\alpha, \phi) = \sum_{k=1}^{\infty} A_k C_k(\alpha) \varphi_k(\alpha, \phi). \quad (38)$$

We can choose initial conditions on a hypersurface  $\alpha = \alpha_0$ . Here, it suffices to fix the values  $\Psi(\alpha_0, \phi)$  and  $\frac{\partial \Psi(\alpha, \phi)}{\partial \alpha}|_{\alpha=\alpha_0}$ . As for the chosen normalizable solution (27)  $\varphi_k(\alpha, \phi)$  vanishes at  $\phi = 0$  for all  $k$  and  $\alpha$ , the wave packet is zero there. This is, of course, independent of the initial conditions. But the classical singularity occurs at  $\phi = 0$ . So out of these solutions, no wave packet can be constructed which does *not* vanish at the classical singularity. Taking  $\alpha$  as an internal time variable, one can calculate the probability distribution,

$$|\Psi|^2(\alpha_0, \phi) = \sum_{l,k} A_k A_l C_k(\alpha_0) C_l(\alpha_0) \varphi_l(\alpha_0, \phi) \varphi_k(\alpha_0, \phi), \quad (39)$$

for each ‘instant of time’  $\alpha_0$ . It is obvious that  $|\Psi|^2(\alpha_0, 0) = 0$  at  $\phi = 0$ . We emphasize that this is a consequence of the choice of (27).

To manifest the elimination of the classical singularity on the quantum level, also expectation values have been employed, see, for example, [7]. Before calculating the expectation value for  $|\phi|$  for this model using the inner product (28), recall that the avoidance of the singularity of the Coulomb potential in ordinary quantum mechanics is caused by a lowest bound on the energy due to quantization. This again leads to a minimal radius for the ‘trajectory’ of the electron.

Analogously to the Coulomb potential in ordinary quantum mechanics, the energy (of the matter component) in our model is also bounded from below. The minimal energy, given by (29) for  $k = 1$ , corresponds to a minimal ‘radius’, that is, to a minimal value for  $|\phi|$ . This is given by

$$\begin{aligned} \langle |\phi_k| \rangle(\alpha) &= [C_k(\alpha)]^2 \frac{3}{2} [Z(\alpha)]^2 k^2 \\ &= \left[ K_0 \left( \frac{1}{\sqrt{6}} \frac{V_\alpha}{\hbar^2 k \kappa} \right) \right]^2 \frac{3\hbar^4}{2V_\alpha^2} k^2, \end{aligned}$$

for  $k = 1$ . The classical singularity lies at  $\alpha = \alpha_*$ . In this case the minimal energy is given by

$$E_1(\alpha_*) = -\frac{V_{\alpha_*}^2}{2\hbar^2}, \quad (40)$$

and the expectation value for  $|\phi|$  is consequently given by  $\langle |\phi_1| \rangle(\alpha_*)$ . The boundedness of the energy here prevents the scalar field to evolve to the singularity,  $|\phi| = 0$ , in this case as well.

Note that for  $\alpha \rightarrow \infty$ , the energy is no longer bounded. In this case  $\langle |\phi_1| \rangle \rightarrow 0$ , cf. (40). Of course, one should keep in mind that the expectation value in quantum cosmology has no interpretation in terms of measurement results as it has in conventional quantum theory.

### E. Construction of wave packets

Apart from the avoidance of the singularity, we want to study semi-classical and quantum regimes of the model. To this end, we construct semi-classical wave packets and study their behaviour. Especially we are interested in the regions of configuration space where these packets spread (if they spread at all).

We want  $\Psi(\alpha_0, \phi)$  to be a Gaussian centered at  $\phi_0$  with width  $\sqrt{\frac{Z_0}{2}}$ , where  $Z_0 \equiv Z(\alpha_0)$ . The center  $\phi_0$  should be the value of the classical trajectory at  $\alpha_0$ . Note that we have two classical solutions,  $\phi_+$  and  $\phi_-$ , see (21).<sup>4</sup> So in fact, we have to construct two Gaussians, one centered at  $\phi_0$ , the other at  $-\phi_0$  and superpose both. Write therefore

$$\Psi(\alpha_0, \phi) = \Psi_-(\alpha_0, \phi) + c_1 \Psi_+(\alpha_0, \phi), \quad (41)$$

where  $\Psi_+$  denotes the part of the wave packet being centered around  $\phi_0$  and  $\Psi_-$  the part centered around  $-\phi_0$  at initial ‘time’  $\alpha_0$ .

The calculation of the wave packet will employ only the WKB solution of (30). With suitable initial conditions, it reads

$$C_k(\alpha) = \left( \frac{e^{6\alpha_0}}{e^{6\alpha}} \right)^{\frac{1}{2}} \exp \left[ -\frac{1}{6} \frac{\tilde{V}_0}{\sqrt{2\hbar^2 k^2}} \sqrt{\frac{6}{\kappa^2}} (e^{6\alpha} - e^{6\alpha_0}) \right]. \quad (42)$$

Introducing  $\tau \equiv e^{6\alpha}$  (and denoting  $\tau_0 \equiv e^{6\alpha_0}$ ),

$$C_k(\tau) = \left( \frac{\tau_0}{\tau} \right)^{\frac{1}{2}} \exp \left[ -\frac{1}{6} \frac{\tilde{V}_0}{\sqrt{2\hbar^2 k^2}} \sqrt{\frac{6}{\kappa^2}} (\tau - \tau_0) \right]. \quad (43)$$

Start with the  $\Psi_+$ -part of the wave packet. We here find the requirement

$$\Psi_+(\alpha_0, \phi) = \sum_{k=1}^{\infty} A_k^+ \varphi_k(\alpha_0, \phi) \stackrel{!}{=} e^{-\frac{(\phi - \phi_0)^2}{Z_0}}. \quad (44)$$

Decomposing the Gaussian into the  $\varphi_k(\alpha_0, \phi)$ , one obtains for the coefficients the somewhat lengthy expression

$$\begin{aligned} A_k^+ &= \frac{N_k}{k} \exp \left[ -\frac{\phi_0^2}{Z_0} + \frac{1}{2Z_0} \left( \frac{1}{2k} - \phi_0 \right)^2 \right] \times \\ &\quad \sum_{m=0}^{k-1} (-1)^m (m+1) \frac{(k!)^2}{(k-m-1)!(m+1)!} \\ &\quad \left( \sqrt{\frac{2}{Z_0} \frac{1}{k}} \right)^m D_{-(m+2)} \left[ \sqrt{\frac{2}{Z_0}} \left( \frac{1}{2k} - \phi_0 \right) \right], \end{aligned} \quad (45)$$

where  $D_m(x)$  denote parabolic cylinder functions. Note that this expansion in  $\varphi_k$  cannot be performed at  $\phi = 0$ . Here,  $\varphi_k(\alpha, \phi = 0) = 0$  for all  $k$  as remarked above.

The amplitude of  $\Psi_-$  is obtained in a similar way (or by just substituting  $-\phi_0$  for  $\phi_0$ ). The solution is

<sup>4</sup> The case with two Gaussians is the most general case. One may, of course, wish to choose only one Gaussian in order to represent only one branch of the classical solutions by a wave packet.



$$A_k^- = \frac{N_k}{k} \exp \left[ -\frac{\phi_0^2}{Z_0} + \frac{1}{2Z_0} \left( \frac{1}{2k} + \phi_0 \right)^2 \right] \times \sum_{m=0}^{k-1} (-1)^m (m+1) \frac{(k!)^2}{(k-m-1)!(m+1)!} \left( \sqrt{\frac{2}{Z_0}} \frac{1}{k} \right)^m D_{-(m+2)} \left[ \sqrt{\frac{2}{Z_0}} \left( \frac{1}{2k} + \phi_0 \right) \right]. \quad (46)$$

So the wave packet is given by

$$\Psi(\alpha, \phi) = \sum_{k=1}^{\infty} [A_k^+ + c_1 A_k^-] C_k(\alpha) \varphi_k(\alpha, \phi). \quad (47)$$

The total probability for the wave packet is calculated via

$$\int d\phi |\Psi|^2 = \frac{\tau_0 \hbar^2}{V_0} \frac{1}{\tau^2} \sum_{k=1}^{\infty} [A_k^+ + c_1 A_k^-]^2 \exp \left( -\frac{1}{3} \frac{\tilde{V}_0}{\sqrt{2\hbar^2 k^2}} \sqrt{\frac{6}{\kappa^2}} (\tau - \tau_0) \right). \quad (48)$$

Probability is thus not conserved with respect to internal ‘time’  $\tau$ , as expected [1]. Choose the normalization of the wave packet such that at  $\alpha_0$ ,  $\int d\phi |\Psi|^2 = 1$ . Then,

$$\Psi(\alpha, \phi) = \frac{1}{C} \sum_{k=1}^{\infty} [A_k^+ + c_1 A_k^-] C_k(\alpha) \varphi_k(\alpha, \phi), \quad (49)$$

where the normalization factor is given by

$$C = \sqrt{\frac{\hbar^2}{\tilde{V}_0 \tau_0} \sum_{k=1}^{\infty} [A_k^+ + c_1 A_k^-]^2}. \quad (50)$$

A plot of the wave packet is shown in Figure 6. We recognize that the wave function is peaked around the two branches of the classical trajectory in configuration space, but goes to zero if the region of the classical big-brake singularity,  $a \rightarrow a_*$ , is approached. In this sense the classical singularity is avoided in the quantum theory. This is a consequence of the choice of the normalizable solution (27), which vanishes at  $\phi = 0$  (the region of the big-brake singularity). Moreover, we find that the wave packet does not spread along the classical trajectory.

#### IV. REMARKS ON BIG-BANG SINGULARITY

##### A. Solution to the Wheeler–DeWitt equation

So far, only the big-brake singularity of the model was considered. But the model possesses a second singularity. Namely, its evolution starts with a big bang: as  $a \rightarrow 0$ ,

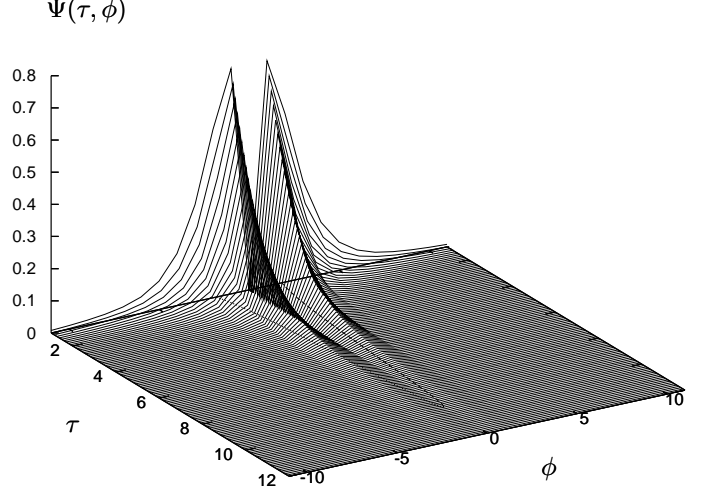


FIG. 6: This plot shows the wave packet. It follows classical trajectories with initial values  $a_0 = 1$  and  $\phi_0 \approx 0.88$ . The classical trajectories are depicted in the  $(\tau, \phi)$ -plane; recall  $\tau = a^6$ . This corresponds to a singularity occurring at  $a_* = 10^{\frac{1}{6}}$ . Parameter values are  $\tilde{V}_0 = 1$ ,  $\hbar = 1$  and  $c_1 = 1$ , cf. (49). Summation was carried out up to  $k = 50$ .

one has  $|\phi| \rightarrow \infty$ . Thus one can approximate the potential by an exponential in the vicinity of this singularity. Choosing units such that  $\kappa^2 = 6$ , one obtains the following form of the Wheeler–DeWitt equation:

$$\frac{\hbar^2}{2} \left( \frac{\partial^2}{\partial \alpha^2} - \frac{\partial^2}{\partial \phi^2} \right) \Psi + \frac{\tilde{V}_0}{2} e^{6\alpha + 3\sqrt{2}|\phi|} \Psi = 0. \quad (51)$$

Introducing coordinates  $z_1 = \alpha + |\phi|$ ,  $z_2 = \alpha - |\phi|$ , the Wheeler–DeWitt equation becomes

$$\hbar^2 \frac{\partial^2}{\partial z_1 \partial z_2} \Psi = f(z_1, z_2) \Psi. \quad (52)$$

One can now find coordinates so that the function on the right-hand side cancels. One is left with

$$\hbar^2 \left( \frac{\partial^2}{\partial u^2} - \frac{\partial^2}{\partial v^2} \right) \Psi + \Psi = 0, \quad (53)$$

where

$$u(\alpha, \phi) = \frac{2\sqrt{\tilde{V}_0}}{3} e^{3(\alpha + \frac{1}{\sqrt{2}}|\phi|)} \left[ \cosh X - \frac{1}{\sqrt{2}} \sinh X \right], \quad (54)$$

$$v(\alpha, \phi) = \frac{2\sqrt{\tilde{V}_0}}{3} e^{3(\alpha + \frac{1}{\sqrt{2}}|\phi|)} \left[ \sinh X - \frac{1}{\sqrt{2}} \cosh X \right], \quad (55)$$

and  $X \equiv 3 \left( |\phi| + \frac{1}{\sqrt{2}} \alpha \right)$ . A solution to this equation can be found from the WKB-ansatz  $\Psi = \int dk A(k) e^{\pm \frac{i}{\hbar} S_{0k}}$ . Inserting this ansatz into (53) yields the Hamilton–Jacobi equation of which an exact solution is given by  $S_{0k} = ku - \sqrt{k^2 - 1}v$ . Of course, the Hamilton–Jacobi equation is also solved by actions with different signs in front of  $u$  and  $v$ . These are obtained from the one chosen above through rotations in the  $(u, v)$ -plane. As  $u > 0$ , only two solutions can be mapped onto each other.

### B. Recovery of classical trajectories

The classical trajectory in the vicinity of the big bang is recovered using the principle of constructive interference  $\frac{dS_{0k}}{dk}|_{k=\bar{k}} = 0$ . For  $\bar{k} = \sqrt{2}$  one finds  $\phi(\alpha) = \pm \frac{1}{\sqrt{2}}\alpha$ . This is just the classical trajectory obtained from (21) in the limit  $|\phi| \gg 1$  with initial condition  $B = \frac{A}{4}$  and fixed  $A$ .

### C. Construction of wave packets

We get the following exact wave-packet solution to the Wheeler–DeWitt equation:

$$\Psi(u, v) = \int dk A(k) \left( C_1 e^{\frac{i}{\hbar}(ku - \sqrt{k^2 - 1}v)} + C_2 \text{ c.c.} \right), \quad (56)$$

where *c.c.* denotes the complex conjugate of the preceeding term. By construction, the classical trajectories can be recovered from this equation through the principle of constructive interference. Choosing as amplitude a Gaussian with width  $\sigma$  centered around  $\bar{k}$ ,

$$A(k) = \frac{1}{(\sqrt{\pi}\sigma\hbar)^{1/2}} e^{-\frac{(k-\bar{k})^2}{2\sigma^2\hbar^2}},$$

and taking  $C_1 = C_2$  for definiteness, one obtains wave packets of the form

$$\psi(u_\ell, v_\ell) \approx C_1 \pi^{1/4} \sqrt{\frac{2\sigma\hbar}{1 - i\sigma^2\hbar S_0''}} \exp\left(\frac{iS_0}{\hbar} - \frac{S_0'^2}{2(\sigma^{-2} - i\hbar S_0'')}\right) + \text{c.c.}, \quad (57)$$

where a Taylor expansion of  $S_{0k}$  has been carried out around  $\bar{k}$  (primes denoting derivatives with respect to  $k$ ) and the terms of the order  $(k - \bar{k})^3$  in the exponent have been neglected. (For simplicity, in this expression  $S_{0k}(\bar{k}) \equiv S_0$ .) This can be done if the Gaussian is strongly peaked around  $\bar{k}$ , that is, if  $\sigma$  is sufficiently small. Since  $S_{0k}'(\bar{k}) = 0$  gives the classical trajectory, the packet is peaked around it.

### D. Singularity avoidance

Due to the fact that  $u > 0$ , two inequivalent actions exist. Apart from the wave packet constructed from  $S_{0k} = ku - \sqrt{k^2 - 1}v$ , one gets a second wave packet constructed from  $S_{0k} = -ku - \sqrt{k^2 - 1}v$ . Moreover, the entire  $(\alpha, \phi)$  plane is mapped into only a quarter of the  $(u, v)$  plane. One would therefore require the wave packet to vanish on the boundary of the physical region. The only solution satisfying this requirement is naturally the trivial one. To get a non-trivial solution, one has to lessen the boundary condition and require  $\Psi = 0$  only at the origin of the  $(u, v)$  plane. The fact that the wave packet does not vanish at the  $u = 0$  and  $v = 0$  line is due to the non-normalizability of the wave packet in both  $\alpha$  and  $\phi$ , which in turn has its origin in the fact that the approximation to the classical trajectory for large  $|\phi|$  has no turning point.

The implementation of the condition of normalizability results in a wave packet which vanishes at the big-bang singularity,  $\Psi \rightarrow 0$  as  $\alpha \rightarrow -\infty$ , and spreads for large  $\alpha$ . This is equivalent to the condition  $\Psi \rightarrow 0$  as  $|\phi| \rightarrow \infty$ . The condition implied for large  $|\phi|$  in the vicinity of the big bang thus implies and justifies the normalization condition imposed in the derivation of the solution to the Wheeler–DeWitt equation in the vicinity of the big brake, cf. (26). We thus impose basically two conditions on the wave function. The first one is that  $\Psi \rightarrow 0$  when  $|\phi| \rightarrow \infty$ , resulting in a normalization condition for the approximate solution in the vicinity of the big-brake singularity and the elimination of the big-bang singularity. The second condition is to require  $\Psi \rightarrow 0$  as  $a \rightarrow \infty$  to ensure the existence of wave packets that follow the classical trajectory. Upon matching the wave function in the two regimes, one would expect quantization conditions as observed e.g. in [30] or [32]. The big-bang singularity does therefore not exist in the quantum theory.

The method employed in this section mirrors the calculation carried out in [15]. The picture one obtains is thus the following. For large  $|\phi|$ , the wave packet vanishes and so does the wave packet for small  $|\phi|$ . In the intermediate region, the packet is peaked around the corresponding approximation to the classical trajectory, cf. Figure 7.

## V. RELATION TO LOOP QUANTUM COSMOLOGY

As discussed in the introduction, there is a whole class of difference operators in the current loop quantum cosmology literature. The ambiguity stems not only from the freedom to choose a factor ordering, but also from the fact that the Hamiltonian constraint contains a curvature

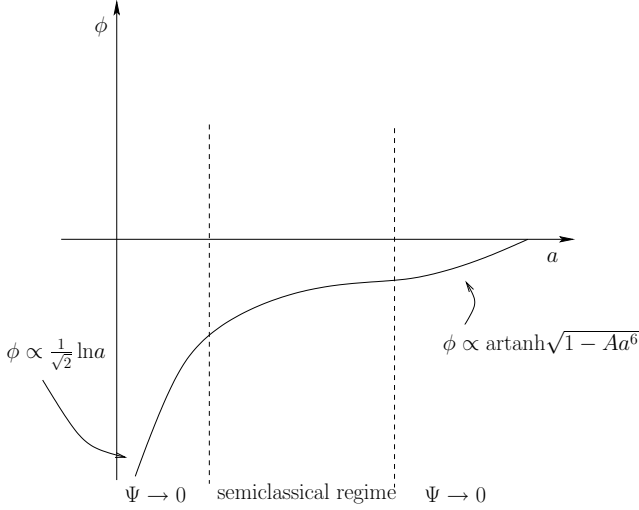


FIG. 7: The different regions of the wave packets and the classical trajectories are shown.

term which, when expressed in terms of holonomies, is given by a limiting procedure. This limiting procedure consists of shrinking an area to zero. But in loop quantum gravity there is a smallest area and thus the limit is heuristically reduced to

$$\text{Area} \rightarrow \Delta \equiv \text{minimal area} . \quad (58)$$

There are at least two ways to implement this. First, one can send the side length of the area to the value  $\mu \rightarrow \mu_0 \equiv \Delta^{\frac{1}{2}}$  [6]. Then  $\mu_0$  is just some number. But on the other hand, one can require that the *physical* length is taken to its minimal value. But the physical length depends on the scale factor and so does  $\bar{\mu}$ ,  $\mu \rightarrow \bar{\mu} \equiv \bar{\mu}(|p|)$ ,  $|p| = a^2$  [7].<sup>5</sup> Depending on which of the two viewpoints is taken, one arrives at a difference equation either in eigenvalues of the triad,  $\mu$ , or in eigenvalues of the volume operator,  $v$ . (As discussed in the introduction, this is more suitably understood as a volume-dependent creation of vertices and thus a refined implementation of the action of the full Hamiltonian constraint.)

The Wheeler–DeWitt equation is recovered in the respective continuum limit. Starting from the same factor-ordering of the difference equation, both versions of it,

the one equidistant in  $\mu$ , the other equidistant in  $v$ , have the same Wheeler–DeWitt limit, meaning they yield the same factor-ordering of the Wheeler–DeWitt equation. As in [6] and [7, 8] different factor orderings have been employed, we comment briefly on both of them here. The question of whether the preceding result persists in loop quantum cosmology can then be reformulated as the question whether the results obtained in Sec. III are robust with respect to a change of factor ordering.

### A. Non-covariant factor ordering

The question here is under which conditions the continuum limit is justified. It is justified if the discreteness of spacetime is negligible compared to the length scales occurring in the model. For large scale factor,  $a \gg \mu_0$ , one can argue that the limit  $\mu_0 \rightarrow 0$  is a sensible approximation. Thus singularity avoidance for large-scale singularities as, for example, the big rip or big brake, in the loop quantum cosmology framework, reduces to singularity avoidance induced by the Wheeler–DeWitt equation.

The Wheeler–DeWitt equation emerging in the continuum limit of the difference equation employed in [6] is

$$\frac{\hbar^2}{2} \left[ \frac{\kappa^2}{6} a^2 \frac{\partial^2 \Psi}{\partial a^2} - \frac{\partial^2 \Psi}{\partial \phi^2} \right] - a^6 \frac{\tilde{V}_0}{|\phi|} \Psi = 0 , \quad (59)$$

which differs from (25) by the choice of factor-ordering. Making the ansatz  $\Psi(a, \phi) = \sum_k A(k) C_k(a) \varphi_k(a, \phi)$  and requiring  $\varphi_k(a, \phi)$  to be a solution of

$$\left( \frac{\hbar^2}{2} \frac{\partial^2}{\partial \phi^2} + a^6 \frac{\tilde{V}_0}{|\phi|} \right) \varphi_k(a, \phi) = -E_k(a) \varphi_k(a, \phi) , \quad (60)$$

one finds as before the solution

$$\varphi_k(x_k) = N_k x_k e^{-\frac{x_k}{2}} L_{k-1}^1(x_k) , \quad (61)$$

where  $x_k = 2\sqrt{-\frac{2E_k(a)}{\hbar^2}}|\phi|$  and  $E_k(a) = -\frac{1}{2\hbar^2 k^2} \tilde{V}_0^2 a^{12}$ . Then the equation for  $C_k(a)$  is given by

$$\frac{d^2 C_k(a)}{da^2} - \frac{6\tilde{V}_0^2}{\hbar^4 k^2 \kappa^2} a^{10} C_k(a) = 0 , \quad (62)$$

which is solved by

$$C_k(a) = c_1 \sqrt{a} J_{\frac{1}{12}} \left( \frac{1}{6} \sqrt{-\frac{6\tilde{V}_0^2}{\hbar^4 k^2 \kappa^2}} a^6 \right) + c_2 \sqrt{a} Y_{\frac{1}{12}} \left( \frac{1}{6} \sqrt{-\frac{6\tilde{V}_0^2}{\hbar^4 k^2 \kappa^2}} a^6 \right) . \quad (63)$$

<sup>5</sup> The interpretation of the area operator in loop quantum gravity is still unclear. The operator itself is not a Dirac observable and thus even in the sense defined by the loop quantum gravity community not an observable (though it can become a Dirac observable when matter is added). In how far the area operator relates to a physical area is thus unsettled.

The complete solution has an analogous form to the quantum geometrodynamical formulation in Sec. III B. The decisive result is that, because only the factor ordering of the *gravitational part* has been changed compared to (25), the solution for  $\varphi_k(\phi, a)$  handles the singularity avoidance in this framework as well.

### B. Covariant factor ordering

The factor ordering in the more recent paper [7, 8] yields the Laplace–Beltrami factor ordering for the Wheeler–DeWitt equation in the continuum limit. As this is the factor ordering we employed throughout this paper, the results of the previous sections carry over to the loop quantum cosmology analysis without alteration. Note, though, that a consistent loop quantization requires a polymer representation of the matter fields as well. This would require a Bohr compactification of  $\phi$  which may bound the approximate potential  $V(\phi) = \frac{V_0}{|\phi|}$  from above. As the vanishing of the wave function at  $\phi = 0$  is related to the divergence of the potential at this point, it is not clear whether the previous results would survive in the polymer representation; namely, it is imaginable that the regularity condition and thus the ensuing condition that  $\varphi_k(\phi = 0, \alpha) = 0$  becomes redundant. This has to be investigated in future publications.

## VI. DISCUSSION AND OUTLOOK

We studied a Friedmann–Lemaître model with a scalar field obeying an ‘anti-Chaplygin’ equation of state. This model classically ends with a big-brake singularity. The singularity stands out because of its negatively diverging second derivative of the scale factor. This works as an infinitely strong ‘brake’, forcing the derivative of the scale factor to go to zero. The evolution of the scale factor stops. Upon quantizing this model in the quantum geometrodynamical framework, we are led to the Wheeler–DeWitt equation. It can be solved in the vicinity of the big-brake singularity. A separation ansatz yields a Schrödinger-type equation for the hydrogen atom for  $\phi$  (which here plays the role of the radius in the quantum mechanical equation). Solutions to this equation vanish at  $\phi = 0$ , which corresponds to the singularity. Thus, independent of the choice of initial conditions, whatever wave packet is constructed out of these solutions, it is condemned to vanish at the singularity. Therefore we can conclude that in this model as well, the large scale, soft, future singularity is removed from the quantum theory.

The same model was also studied in loop quantum cos-

mology. Here, the analysis was restrained to the vicinity of the big-brake singularity. Two different factor-orderings were studied. For both we could corroborate avoidance of the big-brake singularity.

Due to the special form of the potential, we were able to solve the model in the geometrodynamical framework also in the vicinity of the big-bang singularity. The choice of variables enforces a boundary condition which causes the wave function to vanish at the big bang. This singularity is thus also eliminated in the quantum theory. The imposition of boundary conditions on both ends of the evolution, near the big bang and near the big brake, should imply some kind of quantization rule upon matching the wave packets in both regimes. Such a matching has not been carried out.

What are the implications of this singularity removal? Since the wave packet starts to spread when approaching the region where the classical singularity would lurk, this means that the end of the classical evolution is reached. Any information gathering and utilizing system would stop to exist. A similar scenario may happen when the turning point of a classically recollapsing quantum universe is approached [27]. Classical time then comes to an end. The details of such a scenario can, of course, only be discussed if one goes beyond minisuperspace: the treatment of concepts such as entropy and the arrow of time need additional degrees of freedom [1, 28]. We plan to return to this issue in a future publication.

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### APPENDIX A: VALIDITY OF BORN–OPPENHEIMER APPROXIMATION

The Born–Oppenheimer approximation consists in neglecting cross-terms of the form

$$A_{nm} = \int_0^\infty d\phi \, \varphi_n(x_n) \frac{\partial}{\partial \alpha} \varphi_m(x_m) .$$

To be able to give some indication of the quality of the approximation, it is necessary to evaluate these terms. Carrying out the differentiation, one finds

$$A_{nm} = 3 \int_0^\infty d\phi x_n x_m e^{-\frac{x_m + x_n}{2}} L_{n-1}^1(x_n) (L_m^1(x_m) - L_{m-2}^1(x_m)) .$$

This integral can be evaluated using the general formula [34]

$$\begin{aligned} & \int_0^\infty dx e^{-bx} x^a L_n^a(\lambda x) L_m^a(\mu x) \\ &= \frac{\Gamma(m+n+a+1)}{m!n!} \frac{(b-\lambda)^n (b-\mu)^m}{b^{m+n+a+1}} \times \\ & F\left(-m, -n; -m-n-a; \frac{b(b-\lambda-\mu)}{(b-\lambda)(b-\mu)}\right) . \end{aligned}$$

Starting with the first part of the integral in (A1),

$$X_1 \equiv \int_0^\infty d\phi \phi^2 e^{-k\phi} L_{n-1}^1(\lambda\phi) L_m^1(\mu\phi) ,$$

where the short hands  $k \equiv \frac{n+m}{Z(\alpha)nm}$ ,  $\lambda = \frac{2}{Z(\alpha)n}$  and  $\mu = \frac{2}{Z(\alpha)m}$  have been used, one finds

$$\begin{aligned} X_1 &= (-1)^{n-1} \frac{Z(\alpha)^3}{2} m^2 n (m+1)^2 (n+m-1)! (m+1)! \\ & \left(\frac{nm}{m-n}\right)^2 \left(\frac{m-n}{m+n}\right)^{m+n} \times [X_{11} - X_{12} - X_{13}] . \end{aligned}$$

Here,

$$\begin{aligned} X_{11} &= 2 \left(\frac{m-n}{m+n}\right) F\left(-m, -n+1; -m-n; \left(\frac{m+n}{m-n}\right)^2\right) \\ X_{12} &= F\left(-m+1, -n+1; -m-n+1; \left(\frac{m+n}{m-n}\right)^2\right) \\ X_{13} &= \frac{(n+m+1)}{m(m+1)} \frac{(m-n)^2}{(m+n)} \times \\ & F\left(-m-1, -n+1; -m-n-1; \left(\frac{m+n}{m-n}\right)^2\right) . \end{aligned}$$

Similarly, the second part,

$$X_2 \equiv \int_0^\infty d\phi \phi^2 e^{-k\phi} L_{n-1}^1(\lambda\phi) L_{m-2}^1(\mu\phi) ,$$

can be integrated to

$$\begin{aligned} X_2 &= (-1)^{n-1} \frac{Z(\alpha)^3}{2} mn(m-1)^2(m-2)(m+n-3)! \\ & \left(\frac{nm}{m-n}\right)^2 \left(\frac{m-n}{m+n}\right)^{m+n} \\ & \times [X_{21} - X_{22} - X_{23}] , \end{aligned}$$

where

$$\begin{aligned} X_{21} &= 2 \frac{(m+n-2)}{(m-2)} \left(\frac{m-n}{m+n}\right) \\ & F\left(-m+2, -n+1; -m-n+2; \left(\frac{m+n}{m-n}\right)^2\right) \\ X_{22} &= F\left(-m+3, -n+1; -m-n+3; \left(\frac{m+n}{m-n}\right)^2\right) \\ X_{23} &= \frac{(m+n-2)(m+n-1)}{(m-2)(m-1)} \left(\frac{m-n}{m+n}\right)^2 \\ & F\left(-m+1, -n+1; -m-n+1; \left(\frac{m+n}{m-n}\right)^2\right) . \end{aligned}$$

Taking into account the prefactors, one finds

$$A_{nm} = Z(\alpha) 3m \left(\frac{2}{n}\right) \left(\frac{2}{m}\right) \left[ \frac{X_1}{Z(\alpha)^3} - \frac{X_2}{Z(\alpha)^3} \right] .$$

So  $A_{nm} \propto Z(\alpha) \propto a^{-6}$ . For  $a = a_*$  it thus takes its minimal value. This shows that the Born–Oppenheimer approximation is fulfilled best when one approaches the region of the classical singularity.

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